

Pinning of Fermionic Occupation Numbers

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The Pauli exclusion principle is a constraint on the natural occupation numbers of fermionic states. It has been suspected since at least the 1970's, and only proved very recently, that there is a multitude of further constraints on these numbers, generalizing the Pauli principle. Here, we provide the first analytic analysis of the physical relevance of these constraints. We compute the natural occupation numbers for the ground states of a family of interacting fermions in a harmonic potential. Intriguingly, we find that the occupation numbers are almost, but not exactly, pinned to the boundary of the allowed region (*quasi-pinned*). The result suggests that the physics behind the phenomenon is richer than previously appreciated. In particular, it shows that for some models, the generalized Pauli constraints play a role for the ground state, even though they do not limit the ground-state energy. Our findings suggest a generalization of the Hartree-Fock approximation.

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Introduction.— In 1925 the study of atomic transitions led to Pauli's exclusion principle [1]. It states that for identical fermions the occupation number for any quantum state cannot exceed the value 1. By 1926, Dirac [2] and Heisenberg [3] had identified the exclusion principle as a consequence of a much deeper statement: the anti-symmetry of the many-fermion wave function. While anti-symmetry allows one to find the correct solutions to the full many-fermion Schrödinger equation, it does not render the exclusion principle obsolete: In many situations, the latter is sufficient to predict the qualitative behavior of fermionic systems without the need to resort to (often computationally intractable) *ab initio* methods. The *Aufbau* principle for elements in the periodic table serves as a prime example.

This observation motivates the study of generalizations of the exclusion principle, which, maybe surprisingly, exist and exhibit an extremely rich structure [4]. To set the scene, note that the Pauli constraint can be stated succinctly as

$$0 \leq \lambda_i \leq 1 \quad \forall i \quad (1)$$

in terms of the *natural occupation numbers* λ_i , which are the eigenvalues of the 1-particle reduced density operator (1-RDO) ρ_1 , normalized to the particle number N . The utility of the exclusion principle is grounded in the fact that in the ground states of many-fermion systems, one often observes $\lambda_i \approx 0$ or $\lambda_i \approx 1$, which is equivalent to stating that the Hartree-Fock approximation works fairly well in these systems.

It had been observed in the 1970s that there are further linear inequalities respected by the natural occupation numbers as a result of global anti-symmetry [5–7]. One particular example is the so-called Borland-Dennis setting $\wedge^3[\mathcal{H}_6]$ of three fermions and a six dimensional 1-particle Hilbert space \mathcal{H}_6 [7]. Here, the set of constraints is given by

$$\lambda_1 + \lambda_6 = \lambda_2 + \lambda_5 = \lambda_3 + \lambda_4 = 1 \quad (2)$$

$$D^{(6)} := \lambda_5 + \lambda_6 - \lambda_4 \geq 0 \quad (3)$$

on the ordered eigenvalues $\lambda_i \geq \lambda_{i+1}$.

In a ground-breaking work building on recent progress in invariant theory and representation theory, Klyachko exhibited an algorithm for computing *all* such Pauli-like constraints [4, 8]. In fact, his work is part of a more general effort in quantum information theory addressing the *quantum marginal problem* which asks when a given set of single-site reduced density operators (marginals) is compatible in the sense that they arise from a common pure global state (see also [9–12]). The global state may be subject to certain symmetry constraints—one obtains the fermionic case (commonly known as the N -representability problem [13, 14]) by requiring total anti-symmetry under particle exchange. Klyachko showed that for fixed particle number N and dimension d of the 1-particle Hilbert space, the generalized Pauli constraints amount to affine inequalities of the form

$$\kappa_0 + \kappa_1 \lambda_1 + \dots + \kappa_d \lambda_d \geq 0. \quad (4)$$

Geometrically, these constraints define a *convex polytope* $\mathcal{P}_{N,d} \subset \mathbb{R}^d$ of possible spectra (for more details see Appendix A). In general, if a spectral inequality such as (1) or (4) is (approximately) saturated we say that the corresponding spectrum is (quasi-) pinned to its extremum.

The natural question arises as to whether ground states of relevant many-body models saturate some of those inequalities. Strong numerical evidence supporting this conjecture has been presented in [15]. The problem is challenging to address analytically, as one has to not only compute the ground state, but also determine and diagonalize the corresponding 1-RDO.

Here, we present for the first time an analytic analysis. For the ground state of a model of interacting fermions in a harmonic potential, the natural occupation numbers are calculated. We obtain several results. We confirm that for this very natural model, the natural occupation numbers lie indeed close to the boundary of set of allowed ones. The analytic analysis enables us to track the “trajectory” of eigenvalues as a function of the interaction strength between the fermions. What is conceptually also important, is the fact that the eigenvalues never lie *exactly* on the boundary. To see why one could expect the opposite, note that the ground state energy of

a Hamiltonian $H = \sum_{i,j} h^{(i,j)}$ with two-particle terms $h^{(i,j)}$ can be represented as a constrained optimization problem

$$E_{\min} = \min_{\rho_2^{(i,j)}} \sum_{i,j=1}^N \text{tr}[h^{(i,j)} \rho_2^{(i,j)}]$$

where the $\rho_2^{(i,j)}$ are 2-particle density operators that are *compatible* in the sense that they are the reduced densities of some N -fermion state [13, 14]. Since the energy functional is linear, it does not possess an unconstrained minimum. Therefore, E_{\min} will be achieved on the boundary of the set of compatible density operators, where at least one of the compatibility constraints is *active* in the sense that any further minimization would violate it. One way of understanding why a “pinning” effect for the natural occupation numbers is observed, is to posit that the generalized Pauli constraints are among the active physical constraints. While this effect may well occur, we show in this work that *quasi*-pinning appears in natural fermionic systems: the eigenvalue constraints seem to play a role, but are not active in the above sense. The finding suggests that the physics of the phenomenon is richer than previously appreciated. We will return to the physical consequences quasi-pinning has on the structure of wave functions after presenting the calculations for our model system.

The Model.— In order to analyze possible pinning effects analytically, we consider a model of N identical fermions subject to a harmonic external potential and a harmonic interaction term:

$$H = \sum_{i=1}^N \left(\frac{p_i^2}{2m} + \frac{1}{2} m \omega^2 x_i^2 \right) + \frac{1}{2} D \sum_{i,j=1}^N (x_i - x_j)^2. \quad (5)$$

The corresponding eigenvalue problem without any symmetry constraint can easily be solved by transforming the Hamiltonian to the one of decoupled harmonic oscillators. Two eigenfrequencies appear: a non-degenerate one describing the center of mass motion and another $(N-1)$ -fold degenerate frequency associated with the relative motion. The natural length scales corresponding to these eigenmodes are

$$l := \sqrt{\frac{\hbar}{m\omega}}, \quad \tilde{l} := \sqrt{\frac{\hbar}{m\omega\sqrt{1+ND/(m\omega^2)}}}.$$

By rescaling the energy and the length scale, the fermion-fermion coupling constant D can be absorbed by the term $m\omega^2$. Hence the spectrum λ of a 1-RDO corresponding to an eigenstate of H depends only on the relative fermion-fermion interaction strength $\frac{ND}{m\omega^2} = \left(\frac{l}{\tilde{l}}\right)^4 - 1$. In fact, it will prove slightly more convenient to parameterize the coupling using

$$\delta := \ln \left(\frac{l}{\tilde{l}} \right) = \frac{1}{4} \ln \left(1 + \frac{ND}{m\omega^2} \right). \quad (6)$$

Then, in the regime of weak interaction, D and δ are in leading order proportional, $D = \frac{4m\omega^2}{N} \delta + O(\delta^2)$.

To study the physical relevance of the generalized Pauli constraints we restrict the Hamiltonian H to the fermionic

Hilbert space $\wedge^N[\mathcal{H}_\infty]$, with $\mathcal{H}_\infty = L^2(\mathbb{R})$, i.e. we are treating the N particles as fermions (without spin). In [16] H has been diagonalized and the ground state reads in spatial representation ($\vec{x} = (x_1, \dots, x_N)$)

$$\Psi_N(\vec{x}) = \text{const} \times \prod_{1 \leq i < j \leq N} (x_i - x_j) \times \exp \left[-\frac{1}{2N} \left(\frac{1}{l^2} - \frac{1}{\tilde{l}^2} \right) (x_1 + \dots + x_N)^2 - \frac{1}{2} \frac{1}{\tilde{l}^2} \vec{x}^2 \right]. \quad (7)$$

(Note its structural similarity to Laughlin’s ground state wave function describing the fractional quantum Hall effect [17]. Moreover, the polynomial in front of the exponential function is the Vandermonde determinant and by omitting it we obtain the ground state in the bosonic N -particle Hilbert space.)

The spectrum and its properties.— We now outline the calculation of the spectrum $\lambda(\delta)$ as a function of the coupling. We omit details of this tedious but mostly straight-forward computation, presenting the final result, together with some conceptual insights obtained along the way.

The 1-RDO is calculated by integrating out $N-1$ coordinates of the N -fermion state $\rho_N(\vec{x}, \vec{x}') = \Psi_N^*(\vec{x}) \Psi_N(\vec{x}')$. An exercise in Gaussian integration and integration by parts yields

$$\rho_1(x, x') = p(x, x') \exp[-\alpha(x^2 + x'^2) + \beta x x'],$$

where p is a symmetric polynomial of degree $\binom{N}{2}$ in the variables x, x' originating from the Vandermonde determinant in (7), and α and β some constants depending on l, \tilde{l} and N .

If the fermions do not interact with each other, the ground state $|\Psi_N\rangle$ is a single Slater determinant and the spectrum of its 1-RDO is trivial, i.e.

$$\lambda(\delta = 0) = (\underbrace{1, \dots, 1}_N, 0, \dots). \quad (8)$$

The regime of weak interaction can be characterized by the condition $|D| \ll m\omega^2$ or, equivalently, $\delta \approx 0$. We thus employ degenerate perturbation theory to obtain $\lambda(\delta)$ around $\delta = 0$. The reason we employ the parameter δ is that one can prove a duality

$$\lambda_k(\delta) = \lambda_k(-\delta) \quad \forall k \quad (9)$$

relating the spectra for attractive ($\delta < 0$) and repulsive ($\delta > 0$) fermion-fermion interaction (interestingly, that this duality holds is not obvious on the level of ground-state wave functions). This immediately implies that the expansion $\lambda(\delta)$ contains only even order terms, simplifying the perturbation theory.

The solution for $N = 3$ reads:

$$\begin{aligned}
1 - \lambda_1 &= \frac{40}{729}\delta^6 - \frac{1390}{59049}\delta^8 + O(\delta^{10}) \\
1 - \lambda_2 &= \frac{2}{9}\delta^4 - \frac{232}{729}\delta^6 + \frac{3926}{10935}\delta^8 + O(\delta^{10}) \\
1 - \lambda_3 &= \frac{2}{9}\delta^4 - \frac{64}{243}\delta^6 + \frac{81902}{295245}\delta^8 + O(\delta^{10}) \\
\lambda_4 &= \frac{2}{9}\delta^4 - \frac{64}{243}\delta^6 + \frac{73802}{295245}\delta^8 + O(\delta^{10}) \\
\lambda_5 &= \frac{2}{9}\delta^4 - \frac{232}{729}\delta^6 + \frac{3976}{10935}\delta^8 + O(\delta^{10}) \\
\lambda_6 &= \frac{40}{729}\delta^6 - \frac{2200}{59049}\delta^8 + O(\delta^{10}) \\
\lambda_7 &= \frac{80}{2187}\delta^8 + O(\delta^{10}) \\
\lambda_8 &= O(\delta^{10}) \\
&\vdots \\
&\vdots
\end{aligned} \tag{10}$$

Similar results follow for $N = 2$. Note the non-trivial *hierarchy* of the eigenvalues,

$$\lambda_k = c_k \delta^{2k-6} + O(\delta^{2k-4}), \tag{11}$$

for all $k \geq 5$. Moreover, the spectrum λ for δ not too large is very close to the one of a single Slater determinant. For instance, λ_i , $i = 1, 2, 3$ deviate from 1 and λ_j , $j \geq 4$ from 0 only by at most 1 percent if $|\delta| \leq 0.5$. This emphasizes the relevance of the Pauli constraints (1).

Quasi-Pinning by Generalized Pauli Constraints.— Equipped with the explicit solution (10), we can proceed to analyze whether the generalized Pauli constraints play a role for the ground state. While the underlying 1-particle Hilbert space \mathcal{H}_∞ is infinite-dimensional, the scaling (11) implies that the spectrum is strongly concentrated on a low-dimensional subspace, at least for small δ . One can use this fact to deduce statements about the position of the total eigenvalues from truncated information alone.

This can be understood from simple geometric considerations. Let $d < d' < \infty$. Because a d -dimensional 1-particle Hilbert space can be imbedded into any (larger) d' -dimensional one, one sees that the convex polytope $\mathcal{P}_{N,d}$ is nothing but the intersection between $\mathcal{P}_{N,d'}$ and the set of spectra with only d non-zero eigenvalues (see also Appendix B). Hence any facet of $\mathcal{P}_{N,d}$ arises from the intersection of some facet of $\mathcal{P}_{N,d'}$ with the subspace of said spectra. Formally, a facet F' of $\mathcal{P}_{N,d'}$ consists of points saturating a generalized Pauli constraint

$$D'(\lambda) = \kappa_0 + \sum_{i=1}^d \kappa_i \lambda_i + \sum_{i=d+1}^{d'} \kappa_i \lambda_i \geq 0. \tag{12}$$

Denote the first two summands by $D(\lambda^{\text{tr}})$, where $\lambda^{\text{tr}} = (\lambda_i)_{i=1}^d$ is the truncated spectrum. Clearly, $D(\lambda^{\text{tr}}) = 0$ describes the restriction of the facet to the d -dimensional setting. Now assume the truncated spectrum $\lambda^{\text{tr}}(\delta)$ is not pinned, i.e. $D(\lambda^{\text{tr}}(\delta)) > 0$, then the hierarchical scaling (11) implies

$$D'(\lambda(\delta)) = D(\lambda^{\text{tr}}(\delta)) + O(\delta^{2d-4}), \tag{13}$$

which is positive for δ small enough. Hence the full spectrum λ' also fails to be pinned. The case $d' = \infty$ works in the same way, up to some mild assumptions (see Appendix B).

We will now apply these considerations to our model. First, we truncate to 6 dimensions, which has the advantage that the spectral polytope corresponding to $\wedge^3[\mathcal{H}_6]$ is 3-dimensional and can thus be visualized. In a second step, we take a seventh eigenvalue into account. This setting turns out to be strong enough to establish all statements we have mentioned above – namely that the total spectrum is not exactly pinned, but does lie close to the boundary (quasi-pinned).

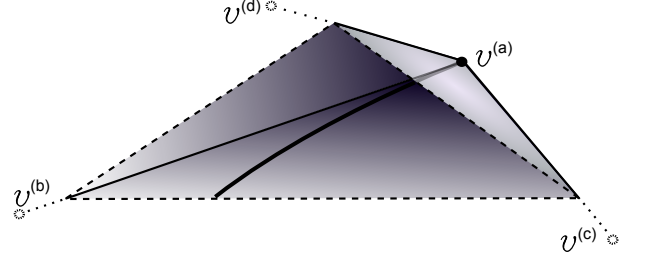


FIG. 1: Spectral “trajectory” $v(\delta)$ (thick line, partially covered by facet, schematic) up to correction of order δ^8 and small part of the polytope \mathcal{P} around vertex $v^{(a)}$ obtained by cutting \mathcal{P} along the dashed lines

The simplest non-trivial setting $\wedge^3[\mathcal{H}_6]$ becomes an appropriate description if $\lambda_7, \lambda_8, \dots \approx 0$. By (11), this condition is fulfilled if δ is small enough that contributions of order δ^8 can be neglected. Choosing λ_4, λ_5 and λ_6 as free parameters according to (2), the corresponding polytope $\mathcal{P}_{3,6}$ effectively reduces [15] to a 3-dimensional polytope $\mathcal{P} \subset \mathbb{R}^3$ with vertices,

$$\begin{aligned}
v^{(a)} &= (0, 0, 0) \quad , \quad v^{(b)} = \left(\frac{1}{2}, \frac{1}{2}, 0\right) \\
v^{(c)} &= \left(\frac{1}{2}, \frac{1}{4}, \frac{1}{4}\right) \quad , \quad v^{(d)} = \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right).
\end{aligned} \tag{14}$$

Hence the vertex $v^{(a)}$ corresponds to single Slater determinants and the 2-facet spanned by $v^{(a)}, v^{(b)}$ and $v^{(c)}$ is defined by $D^{(6)} = 0$, which is here the one of interest and represents exact pinning by constraint (3). We first illustrate schematically our result (10) in Fig. 1. There, the spectral “trajectory”,

$$v(\delta) = (\lambda_4(\delta), \lambda_5(\delta), \lambda_6(\delta)),$$

is shown as a thick line (neglecting effects of order δ^8 and higher). It starts at the vertex $v^{(a)}$ which corresponds to the non-interacting situation $\delta = 0$. When increasing the fermion-fermion interaction, $v(\delta)$ leaves the vertex $v^{(a)}$ and moves along the edge $(v^{(a)}, v^{(b)})$, the distance to $v^{(a)}$ growing as δ^4 . On the finer scale δ^6 , $v(\delta)$ also moves away from the edge but is still *pinned to the boundary* of the polytope, lying on the 2-facet spanned by $v^{(a)}, v^{(b)}$ and $v^{(c)}$. This is the bottom area in Fig. 1, corresponding to the constraint (3).

The pinning seems to disappear if we consider higher orders. From (10), we can infer that the distance to the 2-facet $(v^{(a)}, v^{(b)}, v^{(c)})$ increases as δ^8 ,

$$D^{(6)}(\delta) = \zeta^{(6)} \delta^8 + O(\delta^{10}) \tag{15}$$

with $\zeta^{(6)} = \frac{4510}{59049}$. However, this calculation is inconclusive, as the distance to the boundary is of the same order, δ^8 , as the truncation error (recall (13)).

To resolve the issue, we take another eigenvalue, λ_7 , into account. We thus work in the setting $\wedge^3[\mathcal{H}_7]$ with four constraints $D_i^{(7)} \geq 0$ for $i = 1, \dots, 4$ [4]. This setting is valid as long as $\lambda_8, \lambda_9, \dots \approx 0$ or in other words we neglect terms of order δ^{10} or higher (but in contrast to the setting $\wedge^3[\mathcal{H}_6]$ we include δ^8 -terms). Since the polytope is now 6-dimensional we cannot present our results graphically anymore. The results (10) lead to ($i = 1, 2, 3, 4$)

$$D_i^{(7)} = \zeta_i^{(7)} \delta^8 + O(\delta^{10}), \quad (16)$$

with $\zeta_1^{(7)} = \frac{20}{2187}$, $\zeta_2^{(7)} = \frac{10}{243}$, $\zeta_3^{(7)} = \frac{50}{2187}$, $\zeta_4^{(7)} = \frac{2890}{59049}$. Here in the $\wedge^3[\mathcal{H}_7]$ -analysis, the new result is that all four distances $D_i^{(7)}$ are non-zero to a smaller order, δ^8 , than the error of spectral truncation, δ^{10} . Together with the comments at the beginning of this section, this shows that the absence of pinned spectra is genuine, rather than an artifact of the truncation. Given this, the quasi-pinning found here is surprisingly strong. In particular it exceeds by four additional orders the (quasi-)pinning by Pauli's exclusion principle constraints (1),

$$0 \leq 1 - \lambda_2(\delta), 1 - \lambda_3(\delta), \lambda_4(\delta), \lambda_5(\delta) = \frac{2}{9} \delta^4 + O(\delta^6). \quad (17)$$

Generalizing Hartree-Fock.— In this section, we discuss what conclusions can be drawn about the N -fermion state $|\Psi\rangle$ itself, given information just about the position of the eigenvalues of the corresponding 1-RDO relative to the boundary of the spectral polytope. In this way, quasi-pinned spectra are endowed with a physical significance. To this end, recall the basic fact that the spectrum $\lambda_{\text{Sl}} = (1, \dots, 1, 0, \dots, 0)$ can *only* arise from a Slater determinant $|\Psi\rangle = |1, \dots, N\rangle$. It is well-known that this statement is stable under small deviations: if $\lambda \approx \lambda_{\text{Sl}}$, then $|\Psi\rangle$ is well-approximated by a Slater determinant (see [18] or Appendix D).

For exactly pinned spectra, there is a simple generalization of these observations. In [15], it is stated that constraint (3) can be saturated only by states of the form

$$|\Psi\rangle = \alpha|1, 2, 3\rangle + \beta|1, 4, 5\rangle + \gamma|2, 4, 6\rangle,$$

a fact is dubbed “selection rule” for Slater determinants (see also Appendix C). The general statement reads: if $D(\lambda) \geq 0$ is a generalized Pauli constraint, then $D(\lambda) = 0$ can only be achieved by states $|\Psi\rangle$ which are superpositions of those Slater determinants whose (unordered) spectra also saturate D .

What is more important, a stable version of this statement applying to quasi-pinned states can be found—at least for specific situations. In the Appendix D, we show that for the Borland-Dennis setting, spectra in the vicinity of the facet corresponding to constraint (3) are approximately of the form above. In particular, quasi-pinned states are close to states containing fairly low amounts of multi-partite entanglement as quantified by the Schmidt number [19]. In [20]

a new entanglement measure has been suggested, which, for the Borland-Dennis setting, naturally separates exactly pinned and non-pinned states. We believe that these findings open up a potentially significant avenue for investigating the structure of fermionic ground states via their natural occupation numbers—generalizing a program that has long been carried out for the Hartree-Fock case [18].

We close by speculating that these insights could give rise to improved numerical procedures. The idea is to replace the ground state ansatz of one single Slater determinant by the states corresponding to the points lying on the (quasi-)pinning polytope facet. In contrast to the configuration interaction (CI) methods in quantum chemistry which improve the Hartree-Fock approximation by adding several arbitrary Slater determinants to the Hartree-Fock state our method would add only a few but carefully chosen additional Slater determinants.

Conclusions.— For a natural model of interacting fermions in a harmonic trap we analytically calculated the leading orders of the eigenvalues of the 1-RDO corresponding to the fermionic ground state as function of δ , a measure for the fermion-fermion interaction strength. The investigation of the generalized Pauli constraints has shown that none of them is completely saturated, which might be a generic property of all continuous models of interacting fermions. In particular, the findings show that it is likely extremely challenging to use numerical methods to distinguish between genuinely pinned and mere quasi-pinned states. This underscores the need for analytical analyses, first provided here. On the other hand the pinning up to corrections of order δ^8 we found here is surprisingly strong. In particular it exceed the one by the Pauli exclusion principle constraints (1), which are pinning up to corrections of order δ^4 only.

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Appendix

This appendix is split into four sections. The first one introduces the notation and repeats the solution of the fermionic quantum marginal problem. In the second section we explain how to simplify the pinning analysis by truncating the spectrum. This amounts to the proof of statement (13), a relation connecting polytope distances of the correct and truncated marginal setting. The third section introduces a selection rule, which explains how the structure of a N -fermion state simplifies if its natural occupation numbers are exactly pinned to some Pauli facet and applies it to the Borland-Dennis setting. In the last section we present a modification of this selection rule for the case of only approximate pinning. This then justifies our Hartree-Fock generalization.

A. Notation and Fermionic Quantum Marginal Problem.—

The problem of determining all spectra

$$\lambda = (\lambda_i)_{i=1}^{d'} \quad , \quad 1 \geq \lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_{d'} \geq 0 \quad (18)$$

of 1-particle reduced density operators (1-RDO) ρ_1 arising from some pure N -fermion state $|\Psi\rangle \in \wedge^N[\mathcal{H}_{d'}]$,

$$\rho_1 \equiv N \operatorname{tr}_{N-1}[|\Psi\rangle\langle\Psi|] \quad (19)$$

by tracing out $N-1$ particles, is known as the fermionic quantum marginal problem of the setting $\wedge^N[\mathcal{H}_{d'}]$. Here $d' \in \mathbb{N} \cup \{\infty\}$, $\mathcal{H}_{d'}$ is the d' -dimensional separable 1-particle Hilbert space and we use the trace normalization convention,

$$\operatorname{tr}[\rho_1] = \lambda_1 + \dots + \lambda_{d'} = N, \quad (20)$$

common in quantum chemistry.

For d' finite, the family of possible spectra (we call them compatible w.r.t $\wedge^N[\mathcal{H}_{d'}]$), is described by finitely many independent conditions $\{C_i\}$, the generalized Pauli constraints. Each of them has the form

$$C_i : D_i(\lambda) = \kappa_0 + \kappa_1 \lambda_1 + \dots \kappa_{d'} \lambda_{d'} \geq 0, \quad (21)$$

$\kappa_0, \dots, \kappa_{d'} \in \mathbb{Z}$ and describes a half-space V_i of $\mathbb{R}^{d'}$. These constraints together with the trivial conditions (18) and (20) define the polytope $\mathcal{P}_{N,d'} \subset \mathbb{R}^{d'}$ of possible spectra. In that sense every constraint (21) gives rise to a facet F_i of this polytope,

$$F_i = \{\lambda \in \mathcal{P}_{N,d'} \mid D_i(\lambda) = 0\}. \quad (22)$$

Note that besides these Pauli facets there are also further facets, those corresponding to the trivial constraints (18), but they will not be of interest in our work. Moreover, the quantity $D_i(\cdot)$, which is only defined up to a positive factors, defines after fixing this factor (i.e. the parameters κ_i) a measure for the distance of spectra to the corresponding facet F_i . For the case of d' finite it coincides up to normalization with the Euclidean distance, $\operatorname{dist}_2(\mu, F_i) = \frac{D_i(\mu)}{\|\kappa\|_2}$, $\kappa = (\kappa_1, \dots, \kappa_{d'})$.

For the case $d' = \infty$ the set $\mathcal{P}_{N,\infty}$ of compatible spectra is not explicitly known yet. Nevertheless, for our work we assume that it is also defined by a family of linear inequalities

$$D_j^{(\infty)}(\lambda) = \kappa_0 + \kappa_1 \lambda_1 + \kappa_2 \lambda_2 + \dots \geq 0. \quad (23)$$

The results on truncation of the spectrum and the relation of polytope $\mathcal{P}_{N,d}$ and $\mathcal{P}_{N,d'}$, $d < d'$ finite presented in Appendix B strongly emphasizes that this assumption is justified. Moreover, the involved fact that the l^1 -closure $\overline{\mathcal{P}}_{N,d}$ is convex also suggests this assumption.

Finally, we still make some comments on the meaning of natural orbitals $\{|k\rangle\}$, the eigenvectors of the 1-RDO,

$$\rho_1 = \sum_{k=1}^{d'} \lambda_k |k\rangle\langle k|, \quad (24)$$

and their utility for applications.

These natural orbitals induced by a fixed state $|\Psi\rangle \in \wedge^N[\mathcal{H}_{d'}]$, $d' \in \mathbb{N} \cup \{\infty\}$, define a basis $\mathcal{B}_1 := \{|k\rangle\}_{k=1}^{d'}$ for the 1-particle Hilbert space $\mathcal{H}_{d'}$. For ease of notation we skip the argument Ψ of $|i(\Psi)\rangle$. Basis \mathcal{B}_1 then induces the basis \mathcal{B}_N for $\wedge^N[\mathcal{H}_{d'}]$ of corresponding Slater determinants ($1 \leq i_1 < \dots < i_N \leq d'$)

$$|\mathbf{i}\rangle \equiv |i_1, \dots, i_N\rangle \equiv \mathcal{A}_N[|i_1\rangle \otimes \dots \otimes |i_N\rangle], \quad (25)$$

where \mathcal{A}_N is the anti-symmetrizing operator on the N -particle Hilbert space $\mathcal{H}_{d'}^{\otimes N}$. By expanding $|\Psi\rangle$ w.r.t. to \mathcal{B}_N ,

$$|\Psi\rangle = \sum_{\mathbf{i}} c_{\mathbf{i}} |\mathbf{i}\rangle \quad (26)$$

the natural occupation numbers are given by

$$\lambda_k = \sum_{\mathbf{i}, k \in \mathbf{i}} |c_{\mathbf{i}}|^2. \quad (27)$$

To compare marginal settings of different dimensions, d, d' with $d < d' \leq \infty$ we imbed \mathcal{H}_d into $\mathcal{H}_{d'}$,

$$\operatorname{span}\{|i\rangle\}_{i=1}^d \equiv \mathcal{H}_d \leq \mathcal{H}_{d'} \equiv \overline{\operatorname{span}\{|i\rangle\}_{i=1}^{d'}}, \quad (28)$$

where the closure is only relevant for the case d' infinite. In the same way,

$$\wedge^N[\mathcal{H}_d] \leq \wedge^N[\mathcal{H}_{d'}]. \quad (29)$$

Indeed, according to (26), we find that every state

$$|\Psi\rangle = \sum_{1 \leq i_1 < \dots < i_N \leq d} c_{\mathbf{i}} |\mathbf{i}\rangle \in \wedge^N[\mathcal{H}_d] \quad (30)$$

can be imbedded into $\wedge^N[\mathcal{H}_{d'}]$ by

$$|\Psi'\rangle = \sum_{1 \leq i_1 < \dots < i_N \leq d} c_{\mathbf{i}} |\mathbf{i}\rangle \in \wedge^N[\mathcal{H}_{d'}], \quad (31)$$

and all the other coefficients $c_{\mathbf{i}}$ in (31), those with $i_N > d$, vanish. We used here different symbols for the states $|\Psi\rangle$ and $|\Psi'\rangle$ to distinguish between the two different spaces $\wedge^N[\mathcal{H}_d]$ and $\wedge^N[\mathcal{H}_{d'}]$ to which they belong. This subtle difference is becoming relevant if we determine the natural occupation numbers λ' of $|\Psi'\rangle$ (recall (27)),

$$\lambda' = (\lambda_1, \dots, \lambda_d, \underbrace{0, \dots, 0}_{d'-d}) \quad (32)$$

differing from $\lambda = (\lambda_1, \dots, \lambda_d)$ by additional zeros. In the following, to simplify the notation, we will use the same symbols for mathematical objects and their imbeddings into larger spaces.

B. Truncation of the Spectrum.—

In our work we have determined the “trajectory” of spectra

$$\lambda(\delta) = (\lambda_i(\delta))_{i=1}^\infty \in \mathcal{P}_{3,\infty}, \quad (33)$$

of the 1–RDO corresponding to the ground state of a 3–fermion model with relative fermion-fermion interaction strength δ . The goal was then to show that for δ not too large, $\lambda(\delta)$ is almost but not exactly saturating some of the generalized Pauli constraints of its setting $\wedge^N[\mathcal{H}_\infty]$. Geometrically this means that the vector $\lambda(\delta)$ is very close to some Pauli facet F_i of $\mathcal{P}_{3,\infty}$. In that case we say that the spectrum is quasi-pinned to the facet F_i . Since $\mathcal{P}_{3,\infty}$ is not explicitly known and quite involved (it is described by infinitely many constraints on infinitely many eigenvalues), we have truncated the spectrum and simplified the pinning analysis by considering only the largest d eigenvalues,

$$\lambda^{\text{tr}} = (\lambda_1, \dots, \lambda_d), \quad (34)$$

and analyzed the saturation of the constraints corresponding to the setting $\wedge^3[\mathcal{H}_d]$. The following fact justifies this approach: For $d < d'$ every Pauli facet F of $\mathcal{P}_{N,d}$ is contained in some Pauli facet F' of $\mathcal{P}_{N,d'}$, i.e. F is the intersection of F' with the hyperplane of spectra with only d non-zero eigenvalues. Then, for small $\lambda_{d+1}, \lambda_{d+2}, \dots$, small distance of λ^{tr} to F translates to small distances of λ to F' modulo an error of order of the largest neglected eigenvalue, λ_{d+1} . To illustrate this, we present the example $\wedge^3[\mathcal{H}_6]$, which is one of the two settings studied in our work. There one generalized Pauli constraint reads [4–7]

$$D^{(6)}(\lambda) := 2 - (\lambda_1 + \lambda_2 + \lambda_4) \geq 0. \quad (35)$$

For the setting $\wedge^3[\mathcal{H}_\infty]$ the known constraint [4]

$$D^{(\infty)}(\lambda) = 2 - (\lambda_1 + \lambda_2 + \lambda_4 + \lambda_7 + \lambda_{11} + \lambda_{16} + \dots) \geq 0, \quad (36)$$

coincides with constraint (35) up to a linear combination of eigenvalues $\lambda_7, \lambda_{11}, \lambda_{16}, \dots$, which were neglected in the truncated setting.

A first important step in proving the universality of this relation between polytope distances of correct and truncated setting is the next lemma:

Lemma 1. *Consider the quantum marginal problems of the two settings $\wedge^N[\mathcal{H}_d]$ and $\wedge^N[\mathcal{H}_{d'}]$, $d < d' \in \mathbb{N} \cup \{\infty\}$ and let $\lambda = (\lambda_1, \dots, \lambda_d)$ be a spectrum. Then,*

$$\begin{aligned} &(\lambda_1, \dots, \lambda_d) \text{ compatible w.r.t. } \wedge^N[\mathcal{H}_d] \\ &\Leftrightarrow \\ &(\lambda_1, \dots, \lambda_d, \underbrace{0, \dots, 0}_{d'-d}) \text{ compatible w.r.t. } \wedge^N[\mathcal{H}_{d'}] \end{aligned} \quad (37)$$

For the corresponding polytopes this means

$$\mathcal{P}_{N,d} = \mathcal{P}_{N,d'}|_{\lambda_{d+1}, \lambda_{d+2}, \dots = 0}, \quad (38)$$

the polytope $\mathcal{P}_{N,d'}$ intersected with the hyperplane given by $\lambda_{d+1}, \lambda_{d+2}, \dots = 0$ coincides with $\mathcal{P}_{N,d}$.

Proof. The direction “ \Rightarrow ” was already explained at the end of Section A. To prove “ \Leftarrow ” we show that a state $|\Psi'\rangle$ expanded according to (26),

$$|\Psi'\rangle = \sum_{1 \leq i_1 < \dots < i_N \leq d'} c_i |i\rangle \in \wedge^N[\mathcal{H}_{d'}], \quad (39)$$

with natural occupation numbers $(\lambda_1, \dots, \lambda_d, \underbrace{0, \dots, 0}_s)$ contains only Slater determinants $|i\rangle$, with $i_1, \dots, i_N \leq d$. But this is clear due to (27), which then yields

$$\forall k > d : 0 \stackrel{!}{=} \lambda_k = \sum_{i, k \in i} |c_i|^2. \quad (40)$$

Hence $c_i = 0$ if $i_N > d$. \square

What does Lemma 1 imply for the relation between the families of generalized Pauli constraints of two settings? Let us consider two settings with d, d' finite, $d < d'$. Every constraint D'_j for the setting $\wedge^N[\mathcal{H}_{d'}]$ is linear and hence its restriction

$$\hat{D}'_j(\lambda_1, \dots, \lambda_d) \equiv D'_j(\lambda_1, \dots, \lambda_d, 0, \dots) \geq 0 \quad (41)$$

to the hyperplane defined by $0 = \lambda_{d+1}, \lambda_{d+2}, \dots$ is also a linear constraint in the remaining coordinates $\lambda_1, \dots, \lambda_d$. How is the half space $V_j \subset \mathbb{R}^d$ corresponding to (41) related to the polytope $\mathcal{P}_{N,d}$? Lemma 1 states that

$$\mathcal{P}_{N,d} \subset V_j \quad (42)$$

and

$$\mathcal{P}_{N,d} = \cap_j V_j|_*, \quad (43)$$

where the star $*$ denotes here the restriction to spectra, i.e. ordered and normalized vectors. There are two possible relations between V_j (or $V_j|_*$) and $\mathcal{P}_{N,d}$. They are illustrated in Figure 2 in form of a simplified 2–dimensional picture: There, we consider two half spaces V_1 and V_2 correspond-

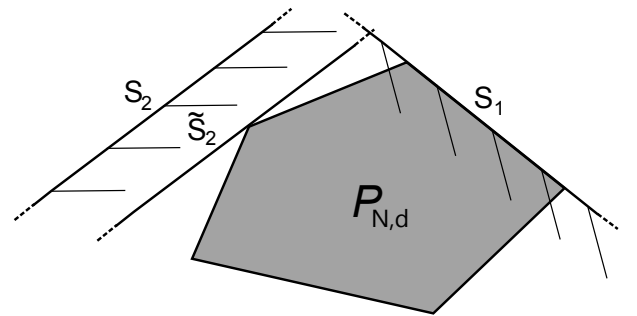


FIG. 2: Polytope $\mathcal{P}_{N,d}$ and two restricted generalized Pauli constraints $\hat{D}_1, \hat{D}_2 \geq 0$ with boundaries S_1, S_2 arising from two constraints $D_1, D_2 \geq 0$ belonging to a higher dimensional marginal settings $\wedge^N[\mathcal{H}_{d'}]$.

ing to the “restricted” constraints $\hat{D}'_1 \geq 0$ and $\hat{D}'_2 \geq 0$ with boundaries S_1 and S_2 and orientation indicated by stripes.

Such hyperplanes can either contain a facet of maximal (example S_1) or lower dimension of $\mathcal{P}_{N,d}$ or they lie outside of $\mathcal{P}_{N,d}$ (example S_2). The third case of a proper intersection is not possible due to Lemma 1. Every constraint D' with boundary S of its restriction \hat{D}' lying outside of $\mathcal{P}_{N,d}$ is a constraint, which is irrelevant for the pinning analysis since it has the form

$$D'(\lambda) = c + \tilde{D}(\lambda^{\text{tr}}) + O(\lambda_{d+1}), \quad (44)$$

where $\tilde{D}(\lambda^{\text{tr}}) \geq 0$ is a constraint of the setting $\wedge^N[\mathcal{H}_d]$ with a boundary shown in Figure 2 as hyperplane \tilde{S}_2 and $c > 0$ is some offset. Hence if the spectrum decays sufficiently fast, constraint D' is not saturated at all due to the offset c and thus irrelevant. Moreover, for every Pauli facet of $\mathcal{P}_{N,d}$ corresponding to some constraint $D > 0$, Lemma 1 guarantees the existence of a constraint $D' > 0$ in the larger setting whose projection \hat{D}' coincides with D . We summarize these insights by stating

Lemma 2. *Given two marginal settings $\wedge^N[\mathcal{H}_d]$ and $\wedge^N[\mathcal{H}_{d'}]$ with $d < d' \in \mathbb{N}$. Every generalized Pauli constraint $D' \geq 0$ of the setting $\wedge^N[\mathcal{H}_{d'}]$ relevant for the pinning analysis is given by a linear modification of some generalized Pauli constraint $D \geq 0$ of the setting $\wedge^N[\mathcal{H}_d]$,*

$$D'(\lambda) = D(\lambda^{\text{tr}}) + O(\lambda_{d+1}). \quad (45)$$

Finally, we remark that for the important case d' infinite effectively the same results holds but one has to deal with one subtlety. Since $\mathcal{P}_{N,\infty}$ is described by infinitely many constraints Lemma 1 guarantees for every constraint $D \geq 0$ of the setting $\wedge^N[\mathcal{H}_d]$, only the existence of a sequence of constraints $D'_j \geq 0$ whose restrictions $\hat{D}'_j \geq 0$ converge to the constraint $D \geq 0$. This means that condition (45) in Lemma 2 holds up to a small error ε ,

$$D'_\varepsilon(\lambda) = \varepsilon + D(\lambda^{\text{tr}}) + O(\lambda_{d+1}), \quad (46)$$

which can be made arbitrarily small by choosing appropriate constraints D'_ε . Hence, to minimize the technical effort we assume in our work that Lemma 2 holds in its original form also for the case d' infinite.

C. Selection Rule.—

In this section we state a selection rule which explains how the structure of the N -fermion state $|\Psi\rangle \in \wedge^N[\mathcal{H}_d]$ simplifies if the spectrum of the corresponding 1-RDO is pinned to some Pauli facet of $\mathcal{P}_{N,d}$. Moreover, we apply it for the setting $\wedge^3[\mathcal{H}_6]$.

Let's consider a state $|\Psi\rangle$ with natural occupation numbers $\lambda = (\lambda_i)_{i=1}^d$ saturating some generalized Pauli constraint

$$D(\lambda) = \kappa_0 + \kappa_1 \lambda_1 + \dots \kappa_d \lambda_d \geq 0. \quad (47)$$

In [15], by introducing the creation and annihilation operator a_k^\dagger, a_k of a fermion in the natural orbital $|k\rangle$ and the particle number operators $N_k \equiv a_k^\dagger a_k$, an important condition is

stated, which $|\Psi\rangle$ in that case satisfies:

$$\hat{D}|\Psi\rangle \equiv (\kappa_0 \text{Id} + \kappa_1 N_1 + \dots \kappa_d N_d) |\Psi\rangle = 0. \quad (48)$$

Applying this condition to the expansion of $|\Psi\rangle$ in Slater determinants induced by the natural orbitals,

$$|\Psi\rangle = \sum_{\mathbf{i}} c_{\mathbf{i}} |\mathbf{i}\rangle \quad (49)$$

it implies *Klyachko's selection rule*, which states that whenever

$$\hat{D}|\mathbf{i}\rangle \neq 0, \quad (50)$$

the corresponding coefficient $c_{\mathbf{i}}$ vanishes. To show the strength of this selection rule we study states in the Borland-Dennis setting. The corresponding Hilbert space $\wedge^3[\mathcal{H}_6]$ has dimension $\binom{6}{3} = 20$ and the generalized Pauli constraints read [4–7]

$$\lambda_1 + \lambda_6, \lambda_2 + \lambda_5, \lambda_3 + \lambda_4 \leq 1 \quad (51)$$

$$D^{(6)} := 2 - (\lambda_1 + \lambda_2 + \lambda_4) \geq 0. \quad (52)$$

The normalization together with the non-negativity of the eigenvalues leads to

$$\lambda_1 + \lambda_6 = \lambda_2 + \lambda_5 = \lambda_3 + \lambda_4 = 1. \quad (53)$$

Hence the constraints in (51) are always saturated and this implies according to (48)

$$\begin{aligned} (\text{Id} - N_1 - N_6) |\Psi\rangle &= 0 \\ (\text{Id} - N_2 - N_5) |\Psi\rangle &= 0 \\ (\text{Id} - N_3 - N_4) |\Psi\rangle &= 0. \end{aligned} \quad (54)$$

Klyachko's selection rule applied to (54) implies that every Slater determinant showing up in the ansatz (49) for $|\Psi\rangle$ is built up by natural orbitals with one index from each set $\{1, 6\}$, $\{2, 5\}$ and $\{3, 4\}$. Those are the 8 states $|1, 2, 3\rangle$, $|1, 2, 4\rangle$, $|1, 3, 5\rangle$, $|1, 4, 5\rangle$, $|2, 3, 6\rangle$, $|2, 4, 6\rangle$, $|3, 5, 6\rangle$ and $|4, 5, 6\rangle$. If the constraint (52) is also saturated the selection rule restricts this family of Slater determinants to the three states $|1, 2, 3\rangle$, $|1, 4, 5\rangle$ and $|2, 4, 6\rangle$ and in that case we find

$$|\Psi_3\rangle = \alpha |1, 2, 3\rangle + \beta |1, 4, 5\rangle + \gamma |2, 4, 6\rangle. \quad (55)$$

D. Quasi-Pinning and modified Selection Rule.—

In this section we show for the Borland-Dennis setting that any state $|\Psi\rangle \in \wedge^3[\mathcal{H}_6]$ whose natural occupation numbers are approximately saturating the corresponding generalized Pauli constraint (52) also fulfill approximately condition (48). We also quantify this relation. This result then guarantees that our Hartree-Fock extension will work for systems exposing strong pinning.

As a warm-up and since we will need the result we first study a simpler question. It is a basic fact that the spectrum $\lambda_{\text{S1}} = (1, \dots, 1, 0, \dots, 0)$ can *only* arise from a Slater determinant $|\Psi\rangle = |1, \dots, N\rangle$. Is this statement stable under small deviations, i.e. $\lambda \approx \lambda_{\text{S1}} \Rightarrow |\Psi\rangle \approx |1, \dots, N\rangle$? Yes, it is true according to

Lemma 3. Consider a state $|\Psi\rangle \in \wedge^N[\mathcal{H}_d]$, let $\{|k\rangle\}_{k=1}^d$ be its natural orbitals and denote the projection operator onto the space spanned by $|1, \dots, N\rangle$ by P_{Sl} . Then,

$$1 - \delta \leq \|P_{\text{Sl}}\Psi\|_{L^2}^2 \leq 1 - \frac{1}{N}\delta, \quad (56)$$

where

$$0 \leq N - (\lambda_1 + \dots + \lambda_N) =: \delta. \quad (57)$$

Proof. We expand the state $|\Psi\rangle$ in Slater determinants induced by natural orbitals (recall Section A),

$$|\Psi\rangle = \sum_{\mathbf{i}} c_{\mathbf{i}} |\mathbf{i}\rangle. \quad (58)$$

We define the operator

$$\hat{S} = N \text{Id} - (a_1^\dagger a_1 + \dots + a_N^\dagger a_N). \quad (59)$$

Since all operators $a_i^\dagger a_i, i = 1, \dots, d$ commute it is clear that \hat{S} has the spectrum $\{0, 1, \dots, N\}$ with eigenstates $|\mathbf{i}\rangle$. The eigenvalue corresponding to $|\mathbf{i}\rangle$ is the number of indices $k \in \mathbf{i}$ not belonging to the set $\{1, \dots, N\}$. We denote the set of indices leading to the eigenvalue k by J_k and find

$$\begin{aligned} \delta &\equiv N - (\lambda_1 + \dots + \lambda_d) \\ &= \langle \Psi | N \text{Id} - (a_1^\dagger a_1 + \dots + a_d^\dagger a_d) | \Psi \rangle \\ &\equiv \langle \Psi | \hat{S} | \Psi \rangle \\ &= \sum_{\mathbf{i}, \mathbf{j} \in J_0 \cup \dots \cup J_N} c_{\mathbf{j}}^* c_{\mathbf{i}} \langle \mathbf{j} | \hat{S} | \mathbf{i} \rangle \\ &= \sum_{\mathbf{i} \in J_0 \cup \dots \cup J_N} |c_{\mathbf{i}}|^2 \langle \mathbf{i} | \hat{S} | \mathbf{i} \rangle. \end{aligned} \quad (60)$$

Since for $\mathbf{i} \in J_k$,

$$\langle \mathbf{i} | \hat{S} | \mathbf{i} \rangle = k \quad (61)$$

we find

$$\delta = \sum_{k=0}^N \sum_{\mathbf{i} \in J_k} |c_{\mathbf{i}}|^2 k \geq \sum_{k=1}^N \sum_{\mathbf{i} \in J_k} |c_{\mathbf{i}}|^2 \quad (62)$$

and alternatively also

$$\delta \leq N \sum_{k=1}^N \sum_{\mathbf{i} \in J_k} |c_{\mathbf{i}}|^2. \quad (63)$$

The normalization of $|\Psi\rangle$, $\sum_{\mathbf{i}} |c_{\mathbf{i}}|^2 = 1$ yields ($J_0 = \{(1, 2, \dots, N)\}$ contains only one element)

$$\frac{\delta}{N} \leq 1 - |c_{(1, \dots, N)}|^2 \leq \delta. \quad (64)$$

and thus

$$1 - \delta \leq |c_{(1, \dots, N)}|^2 \leq 1 - \frac{1}{N}\delta. \quad (65)$$

Now, we come back to the original question. We first state the mathematical result and present the proof afterwards.

Theorem 4. Given a state $|\Psi\rangle \in \wedge^3[\mathcal{H}_6]$ with natural occupation numbers $(\lambda_k)_{k=1}^6$. Let P be the projection operator onto the subspace spanned by the states $|1, 2, 3\rangle, |1, 4, 5\rangle, |2, 4, 6\rangle$, which corresponds to exact pinning of $D^{(6)} = \lambda_5 + \lambda_6 - \lambda_4 \geq 0$ (recall (55)). Then as long as

$$\delta \equiv 3 - \lambda_1 - \lambda_2 - \lambda_3 \leq \frac{1}{4} \quad (66)$$

(which means nothing else but being not too far away from the spectrum $\lambda_{\text{Sl}} = (1, 1, 1, 0, 0, 0)$ of a single Slater determinant) we find

$$1 - \chi_\delta D^{(6)} \leq \|P\Psi\|_2^2 \leq 1 - \frac{1}{2}D^{(6)}, \quad (67)$$

with

$$\chi_\delta \equiv \frac{1 + 2\delta}{1 - 4\delta}. \quad (68)$$

Proof. In Section C we concluded that $|\Psi\rangle$ has the form

$$\begin{aligned} |\Psi\rangle &= \alpha|1, 2, 3\rangle + \beta|1, 2, 4\rangle + \gamma|1, 3, 5\rangle \\ &\quad + \delta|2, 3, 6\rangle + \nu|1, 4, 5\rangle + \mu|2, 4, 6\rangle \\ &\quad + \xi|3, 5, 6\rangle + \zeta|4, 5, 6\rangle, \end{aligned} \quad (69)$$

with natural orbitals $\{|k\rangle\}_{k=1}^6$. Since the corresponding 1-RDO is diagonal w.r.t. $\{|k\rangle\}_{k=1}^6$,

$$\langle k | \rho_1 | l \rangle = \delta_{kl} \lambda_k, \quad (70)$$

we find (recall (27))

$$\lambda_4 = |\beta|^2 + |\nu|^2 + |\mu|^2 + |\zeta|^2 \quad (71)$$

$$\lambda_5 = |\gamma|^2 + |\nu|^2 + |\xi|^2 + |\zeta|^2 \quad (72)$$

$$\lambda_6 = |\delta|^2 + |\mu|^2 + |\xi|^2 + |\zeta|^2 \quad (73)$$

The goal is now to show that the coefficients $\beta, \gamma, \delta, \xi$ and ζ are small, i.e.

$$\begin{aligned} \|P\Psi\|_{L^2}^2 &= |\alpha|^2 + |\mu|^2 + |\nu|^2 \\ &= 1 - (|\beta|^2 + |\gamma|^2 + |\delta|^2 + |\xi|^2 + |\zeta|^2) \end{aligned} \quad (74)$$

is close to 1, whenever (52), which here reads

$$D^{(6)} = -|\beta|^2 + |\gamma|^2 + |\delta|^2 + 2|\xi|^2 + |\zeta|^2, \quad (75)$$

is approximately saturated. First we observe

$$\begin{aligned} \|P\Psi\|_{L^2}^2 &\leq 1 - \frac{1}{2}(|\beta|^2 + |\gamma|^2 + |\delta|^2 + 2|\xi|^2 + |\zeta|^2) \\ &\leq 1 - \frac{1}{2}(-|\beta|^2 + |\gamma|^2 + |\delta|^2 + 2|\xi|^2 + |\zeta|^2) \\ &= 1 - \frac{1}{2}D^{(6)}, \end{aligned} \quad (76)$$

□

which is the upper bound for $\|P\Psi\|_{L^2}^2$ in Theorem 4.

To derive the lower bound note the essential difference in (75) and (76), the sign of the term $|\beta|^2$. To get rid of this we write $|\beta|^2 = -\chi|\beta|^2 + (1+\chi)|\beta|^2$, $\chi > 0$ and estimate $(1+\chi)|\beta|^2$ in terms of $|\gamma|^2, |\delta|^2, |\xi|^2, |\zeta|^2$. For this observe that (70) in particular implies

$$0 = \langle 4|\rho_1|3 \rangle = \bar{\alpha}\beta + \bar{\gamma}\nu + \bar{\delta}\mu + \bar{\xi}\zeta, \quad (77)$$

which leads by the triangle inequality, the identity $(A+B+C)^2 \leq 3(A^2+B^2+C^2)$ and $|\mu|^2, |\nu|^2, |\xi|^2, |\zeta|^2 \leq 1-|\alpha|^2$ to

$$\begin{aligned} |\beta|^2 &= \left| \frac{1}{\bar{\alpha}} (\bar{\gamma}\nu + \bar{\delta}\mu + \bar{\xi}\zeta) \right|^2 \\ &\leq \frac{1}{|\alpha|^2} (|\gamma||\nu| + |\delta||\mu| + |\xi||\zeta|)^2 \\ &\leq \frac{3}{|\alpha|^2} (|\gamma|^2|\nu|^2 + |\delta|^2|\mu|^2 + |\xi|^2|\zeta|^2) \\ &\leq \frac{3(1-|\alpha|^2)}{|\alpha|^2} \left(|\gamma|^2 + |\delta|^2 + \frac{1}{3}(2|\xi|^2 + |\zeta|^2) \right) \end{aligned} \quad (78)$$

Now, for all $s, r \geq 0$ we find by using (78)

$$\begin{aligned} |\beta|^2 + |\gamma|^2 + |\delta|^2 + |\xi|^2 + |\zeta|^2 &\leq (1-r)|\beta|^2 + |\gamma|^2 + |\delta|^2 + (1+s)(2|\xi|^2 + |\zeta|^2) + r|\beta|^2 \\ &\leq (1-r)|\beta|^2 + |\gamma|^2 + |\delta|^2 + (1+s)(2|\xi|^2 + |\zeta|^2) \\ &\quad + \frac{3r(1-|\alpha|^2)}{|\alpha|^2} \left(|\gamma|^2 + |\delta|^2 + \frac{1}{3}(2|\xi|^2 + |\zeta|^2) \right) \\ &= (1-r)|\beta|^2 + \left(1 + \frac{3r(1-|\alpha|^2)}{|\alpha|^2} \right) (|\gamma|^2 + |\delta|^2) \\ &\quad + \left(1 + s + \frac{r(1-|\alpha|^2)}{|\alpha|^2} \right) (2|\xi|^2 + |\zeta|^2). \end{aligned} \quad (79)$$

By choosing

$$r = \frac{2|\alpha|^2}{4|\alpha|^2 - 3} \quad (80)$$

$$s = \frac{4(1-|\alpha|^2)}{4|\alpha|^2 - 3} \quad (81)$$

the last expression in (79) coincides with $D^{(6)}$ up to a global factor χ . Both parameters r, s are non-negative as long as $|\alpha|^2 \geq \frac{3}{4}$. Finally, this leads to

$$\begin{aligned} \|P\Psi\|_{L^2}^2 &= 1 - (|\beta|^2 + |\gamma|^2 + |\delta|^2 + |\xi|^2 + |\zeta|^2) \\ &\geq 1 - (r-1)D^{(6)} \\ &\equiv 1 - \chi_{1-|\alpha|^2} D^{(6)}, \end{aligned} \quad (82)$$

with

$$\begin{aligned} \chi_{1-|\alpha|^2} \equiv r-1 &= \frac{3-2|\alpha|^2}{4|\alpha|^2-3} \\ &= \frac{1+2(1-|\alpha|^2)}{1-4(1-|\alpha|^2)}. \end{aligned} \quad (83)$$

Lemma 3 states $|\alpha|^2 \geq 1-\delta$ and since χ is monotonously increasing, $\chi_{1-|\alpha|^2} \leq \chi_\delta$, which finishes the proof. \square

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